

Geometric Momentum for a Particle on a Curved Surface

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Abstract

When a two-dimensional curved surface is conceived as a limiting case of a curved shell of equal thickness d , where the limit $d \rightarrow 0$ is then taken, the well-known *geometric potential* is induced by the kinetic energy operator, in fact by the second order partial derivatives. Applying this confining procedure to the momentum operator, in fact to the first order partial derivatives, we find the so-called *geometric momentum* instead. This momentum is compatible with the Dirac's canonical quantization theory on system with second-class constraints. The distribution amplitudes of the geometric momentum on the spherical harmonics are analytically determined, and they are experimentally testable for rotational states of spherical molecules such as C_{60} .

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INTRODUCTION The affirmative experimental evidence in 2010¹ of the *geometric potential* firstly explored in 1971² and fundamentally finished in 1981³ and with correct inclusion of electromagnetic field in 2008⁴ etc.⁵ is a groundbreaking advance of quantum mechanics applied for curved nanostructures, starting from the three dimensional (3D) bulk system and then reducing it to a 2D surface one.²⁻⁵ This success echoes a historical footnote in Dirac's *Principle* on the canonical quantization assumption that "is found in practice successful only when applied with the dynamic coordinates and momenta referring to a Cartesian system of axes and not to more general curvilinear coordinates."⁶ However, the classic work by Jensen, Koppe² and da Costa³ hides an important physical and mathematical message when dealing with derivatives on a 2D curved surface S : There is a noninterchangeability of order of taking two limits. Explicitly, when the 2D curved surface is conceived as a limiting case of a curved shell of equal thickness d , where the limit $d \rightarrow 0$ is then taken, great discrepancies present as firstly taking limit $d \rightarrow 0$ then defining the derivatives on the surface, and as firstly defining derivatives in bulk then letting $d \rightarrow 0$. The second order is named as the *confining procedure* for studying motion on 2D surface embedded in 3D.⁴ For the former order, the quantum kinetic energy operator is hypothesized to be proportional to Laplace-Beltrami operator Δ_{LB} on the surface:⁷

$$T = -\frac{\hbar^2}{2\mu}\Delta_{LB}, \quad (1)$$

whereas for the latter order, we have following form of the kinetic energy operator T instead:²⁻⁴

$$T = -\frac{\hbar^2}{2\mu}\Delta_{LB} - \frac{\hbar^2}{2\mu}(M^2 - K), \quad (2)$$

where M is the mean curvature and K is the gaussian curvature, and the excess term is called *geometric potential* V_{gp} ,^{1,4}

$$V_{gp} = -\frac{\hbar^2}{2\mu}(M^2 - K). \quad (3)$$

The experimental verification of this potential implies that the original Laplace-Beltrami operator Δ_{LB} on the 2D surface may not be enough unless a term $(M^2 - K)$ is included,^{1,8}

$$\Delta_{LB} \rightarrow \Delta_{LB} + (M^2 - K). \quad (4)$$

For avoiding confusion, we adhere to the convention in mathematics where the Laplace operator ∇^2 acting on a function is defined by the divergence of the gradient of the function

in flat space: $\nabla^2 \equiv \nabla \cdot \nabla$, while the Laplace-Beltrami operator Δ_{LB} is a generalization of the Laplace operator on surface under consideration.

The noninterchangeability of calculus order must be fundamentally associated with the gradient ∇ , or the momentum operator $\mathbf{p} = -i\hbar\nabla$, which has not explored before. On the other hand, we must mention an entirely independent development on the quantization of the momentum on 2D surface embedded in 3D flat space,⁹ and the momentum is found to assume the following form,

$$\mathbf{p} = -i\hbar(\mathbf{r}^\mu\partial_\mu + M\mathbf{n}), \quad (5)$$

where we use the tensor covariant and contravariant components and the Einstein summation convention, and

$$\mathbf{r}(q^1, q^2) = (x(q^1, q^2), y(q^1, q^2), z(q^1, q^2)) \quad (6)$$

is the position vector on the surface S parametrized by (q^1, q^2) denoted by q^μ and q^ν with lowercase greek letters μ, ν taking values 1, 2, and $\mathbf{r}^\mu = g^{\mu\nu}\mathbf{r}_\nu = g^{\mu\nu}\partial_\nu\mathbf{r} = g^{\mu\nu}\partial\mathbf{r}/q^\nu$ with $g_{\mu\nu} = \partial_\mu\mathbf{r} \cdot \partial_\nu\mathbf{r}$ being the metric tensor. At this point \mathbf{r} , $\mathbf{n} = (n_x, n_y, n_z)$ is the normal and $M\mathbf{n}$ symbolizes the mean curvature vector field, a geometric invariant.⁹

The first aim of the present study is to show that the application of the same confining procedure pioneered by Jensen, Koppe² and da Costa³ to operator $\mathbf{p} = -i\hbar\nabla$ that holds true in bulk automatically results in $\mathbf{p} = -i\hbar(\mathbf{r}^\mu\partial_\mu + M\mathbf{n})$ (5) on the surface. So, analogue to the name *geometric potential* we can call $\mathbf{p} = -i\hbar(\mathbf{r}^\mu\partial_\mu + M\mathbf{n})$ (5) *geometric momentum* (GM). Because $\mathbf{r}(q^1, q^2)$ (6) in mathematics offers the so-called standard parametrization of the 2D surface, the corresponding GM (5) should offer proper description of the momentum. If simply denoting the gradient operator $\mathbf{r}^\mu\partial_\mu$ ¹⁰ on the surface by $\nabla_{//}$, Eq. (5) implies following correspondence,

$$\nabla_{//} \rightarrow \nabla_{//} + M\mathbf{n}. \quad (7)$$

On a surface, is there a component $M\mathbf{n}$ normal to it? This result (7) is somewhat contrary to what physical intuition or common sense would indicate. But it is the case as examined in 3D flat space.

GEOMETRIC MOMENTUM AS A CONSEQUENCE OF CONFINING PROCEDURE To prove the GM (5), we utilize exactly the same manner how to derive the geometric potential.²⁻⁴ For ease of the comparison, we use similar set of symbols as Ferrari and Cuoghi who recently build up a theoretical framework with geometric potential when the electromagnetic field is

present.⁴ The lowercase Latin letters i, j, k stand for the 3D indices and assume the values 1, 2, 3, e.g., (x_i, p_j) for the position and momentum. Position specified by (q^1, q^2, q^3) can be understood as description of the position in the curvilinear coordinates parameterizing a manifold. The original 2D surface $\mathbf{r}(q^1, q^2)$ is considered as a more realistic 3D shell whose equal thickness d is negligible in comparison with the dimension of the whole system. The position \mathbf{R} within the shell in the vicinity of the surface S can be parametrized as with $0 \leq q^3 \leq d$,

$$\mathbf{R}(q^1, q^2, q^3) = \mathbf{r}(q^1, q^2) + q^3 \mathbf{n}(q^1, q^2). \quad (8)$$

The gradient operator ∇ in 3D flat space, expressed in the curvilinear coordinates, takes following form,¹⁰

$$\nabla = \mathbf{r}^\mu \partial_\mu + \mathbf{n} \partial_{q^3}. \quad (9)$$

The relation between the 3D metric tensor G_{ij} and the 2D one $g_{\mu\nu}$ is given by,^{3,4}

$$\begin{aligned} G_{ij} &= g_{\mu\nu} + [\alpha g + (\alpha g)^T]_{\mu\nu} q^3 + (\alpha g \alpha^T)_{\mu\nu} (q^3)^2, \\ G_{\mu 3} &= G_{3\mu} = 0, \quad G_{33} = 1, \end{aligned} \quad (10)$$

where $\alpha_{\mu\nu}$ is the Weingarten curvature matrix for the surface, and $M = -\text{Tr}(\alpha)/2$, and $K = \det(\alpha)$.³ The covariant Schrödinger equation for particles moving within a thin shell of thickness d in 3D is, with both the vector potential V and the electric potential \mathbf{A} applied,⁴

$$i\hbar \frac{\partial}{\partial t} \psi(\mathbf{q}, t) = -\frac{\hbar^2}{2m} G^{ij} D_i D_j \psi(\mathbf{q}, t) + QV \psi(\mathbf{q}, t), \quad (11)$$

where Q is the charge of the particle and $D_j = \nabla_j - (iQ/\hbar)A_j$ with A_j being the covariant components of the vector potential \mathbf{A} . Defining the scalar potential $A_0 = -V$, we can define a gauge covariant derivative for the time variable as $D_0 = \partial_t - iQ A_0/\hbar$, and rewrite Eq.(11) as,⁴

$$i\hbar D_0 \psi = -\frac{\hbar^2}{2m} G^{ij} D_i D_j \psi. \quad (12)$$

This equation is evidently gauge invariant with respect of the following gauge transformations:⁴

$$A_j \rightarrow A'_j = A_j + \partial_j \gamma; \quad A_0 \rightarrow A'_0 = A_0 + \partial_t \gamma; \quad \psi \rightarrow \psi' = \psi e^{iQ\gamma/\hbar}, \quad (13)$$

where γ is a scalar function.

Two important facts regarding the wave functions will be needed. 1, the normalization of the wave functions remains whatever coordinates are used, and we have with transformation

of volume element $d^3\mathbf{x} = \sqrt{G}d^3\mathbf{q}$,⁴

$$\int |\psi(\mathbf{x}, t)|^2 d^3\mathbf{x} = \int |\psi(\mathbf{q}, t)|^2 \sqrt{G}d^3\mathbf{q} = 1, \quad (14)$$

where^{3,4}

$$G = \det(G_{ij}) = g \left(1 - 2Mq^3 + K(q^3)^2\right)^2. \quad (15)$$

2, an advantage of the curvilinear coordinates is the accessibility of the separability of the wave function $\psi(\mathbf{q}, t)$ in (11) or (12) as,^{3,4}

$$\psi(\mathbf{q}, t) = \frac{\chi(q^1, q^2, t)}{\sqrt{1 - 2Mq^3 + K(q^3)^2}} \varphi(q^3, t), \quad (16)$$

and it is guaranteed with suitable choice of gauge for γ such that $A'_3 = 0$,⁴

$$\gamma(q^1, q^2, q^3) = - \int_0^{q^3} A_3(q^1, q^2, q) dq. \quad (17)$$

Combining these two facts, we have two conservations of norm from (14),

$$\oint |\chi(q^1, q^2, t)|^2 \sqrt{g} dq^1 dq^2 = 1, \quad (18)$$

$$\text{and } \int_0^d |\varphi(q^3, t)|^2 dq^3 = 1. \quad (19)$$

We are now ready to examine the gradient operator ∇ (9) acting on the $\psi(\mathbf{q}, t)$ and the result is,

$$\begin{aligned} \nabla \psi(\mathbf{q}, t) &= \mathbf{r}^\mu \partial_\mu \psi(\mathbf{q}, t) + \mathbf{n} \frac{M + q^3 K}{(1 - 2Mq^3 + K(q^3)^2)^{3/2}} \chi(q^1, q^2, t) \varphi(q^3, t) \\ &\quad + \mathbf{n} \frac{\chi(q^1, q^2, t)}{\sqrt{1 - 2Mq^3 + K(q^3)^2}} \partial_{q^3} \varphi(q^3, t). \end{aligned} \quad (20)$$

Then taking limit $d \rightarrow 0$, we have,

$$\nabla \psi(\mathbf{q}, t) = (\mathbf{r}^\mu \partial_\mu + M\mathbf{n}) \psi(\mathbf{q}, t) + \mathbf{n} \chi(q^1, q^2, t) \partial_{q^3} \varphi(q^3, t), \quad (21)$$

which implies that the gradient operator ∇ can be decomposed into two separate parts, one is (q^1, q^2) dependent part $(\mathbf{r}^\mu \partial_\mu + M\mathbf{n})$ and another the q^3 -derivative part $\mathbf{n} \partial_{q^3}$, corresponding to the decomposition of the Schrödinger equation into two Schrödinger ones determining $\chi(q^1, q^2, t)$ and $\varphi(q^3, t)$ respectively.⁴ Paying attention to the motion on the surface only, we have the resultant operator $\mathbf{r}^\mu \partial_\mu + M\mathbf{n}$ (7). In fact, with proper choice of the confining

potential $V(q^3)$ in the confining procedure,^{3,4} we can require that $\int_0^d \varphi^*(q^3, t) \partial_{q^3} \varphi(q^3, t) dq^3 = 0$. So, after performing an integration of operator ∇ in (21) over perpendicular interval $[0, d]$ as $\int_0^d \varphi^*(q^3, t) \nabla \varphi(q^3, t) dq^3$, only the surface part $(\mathbf{r}^\mu \partial_\mu + M\mathbf{n})$ (7) survives.

The gauge invariance of the momentum operator $\mathbf{p} = -i\hbar(\mathbf{r}^\mu \partial_\mu + M\mathbf{n}) - Q\mathbf{A}$ is assured in the presence of the vector potential \mathbf{A} with 3D gauge $A_3 = 0$ being pre-imposed. Under 2D gauge transformation: $\mathbf{A} \rightarrow \mathbf{A}' = \mathbf{A} + \mathbf{r}^\mu \partial_\mu \gamma$ with $\gamma = \gamma(q^1, q^2)$ and $\psi \rightarrow \psi' = e^{iQ\gamma/\hbar} \psi$, we have $\mathbf{p}\psi \rightarrow \mathbf{p}'\psi' = e^{iQ\gamma/\hbar} \mathbf{p}\psi$,

$$\begin{aligned} \mathbf{p}'\psi' &= (-i\hbar(\mathbf{r}^\mu \partial_\mu + M\mathbf{n}) - Q(\mathbf{A} + \mathbf{r}^\mu \partial_\mu \gamma)) \psi e^{iQ\gamma/\hbar} \\ &= e^{iQ\gamma/\hbar} (-i\hbar(\mathbf{r}^\mu \partial_\mu + M\mathbf{n}) - Q\mathbf{A}) \psi \\ &= e^{iQ\gamma/\hbar} \mathbf{p}\psi. \end{aligned} \quad (22)$$

So far, we also understand why there is no direct connection between $\Delta_{LB} + (M^2 - K)$ and $\nabla_{//} + M\mathbf{n}$ such as in 3D flat space $\nabla^2 \equiv \nabla \cdot \nabla$. For reaching $\Delta_{LB} + (M^2 - K)$, we have to start from the Laplace operator in flat 3D space $\nabla^2 = (\mathbf{r}^\mu \partial_\mu + \mathbf{n} \partial_{q^3}) \cdot (\mathbf{r}^\mu \partial_\mu + \mathbf{n} \partial_{q^3}) = \Delta_{LB} + M \partial_{q^3} + \partial_{q^3}^2$, then resort to the confining procedure.

GEOMETRIC MOMENTUM IN DIRAC'S THEORY During 1950's and 1960's, Dirac¹¹ establishes a theory for constrained motion instead follows the routine paradigm of quantization hypothesis of kinetic energy $T = -\hbar^2(2\mu)\Delta_{LB}$ on the curved surface. Recalling his famous footnote,⁶ we can reasonably infer that if his understanding of canonical quantization is self-consistent and indeed insightful, the geometric momentum (5) must be a natural realization of the momentum in the Dirac's canonical quantization for a system with second-class constraints. The second aim of the present study is to illustrate that it is really the case.

For the constrained motion on the surface S (6), Dirac's theory gives for the commutators:¹²⁻¹⁵

$$[x_i, p_j] = i\hbar(\delta_{ij} - n_i n_j), \quad [\mathbf{r}, T] = i\hbar \frac{\mathbf{p}}{m}. \quad (23)$$

The verification of the first commutator whose tensor form is $[\mathbf{r}, \mathbf{p}] = i\hbar(\overset{\rightarrow}{\mathbf{I}} - \mathbf{n}\mathbf{n})$ needs an identity for the second-rank tensor as $\overset{\rightarrow}{\mathbf{I}} = \mathbf{n}\mathbf{n} + \mathbf{r}^\mu \mathbf{r}_\mu$ whose proof is straightforward. In fact, the tensor form of the commutator $[\mathbf{r}, \mathbf{p}] \equiv \mathbf{r}\mathbf{p} - \mathbf{p}\mathbf{r}$ gives:

$$[\mathbf{r}, \mathbf{p}] \equiv -i\hbar[\mathbf{r}, (\mathbf{r}^\mu \partial_\mu + M\mathbf{n})] = i\hbar \mathbf{r}^\mu \mathbf{r}_\mu = i\hbar(\overset{\rightarrow}{\mathbf{I}} - \mathbf{n}\mathbf{n}). \quad (24)$$

The second commutator is evident with use of a formula $\nabla^2 \mathbf{r} = 2M\mathbf{n}$,¹⁰

$$\begin{aligned}
[\mathbf{r}, T] &= -\frac{\hbar^2}{2m}[\mathbf{r}, \Delta_{LB}] = \frac{\hbar^2}{2m} \left(\frac{1}{\sqrt{g}}(\partial_\mu g^{\mu\nu} \sqrt{g} \partial_\nu \mathbf{r}) + 2(\partial^\nu \mathbf{r}) \partial_\nu \right) \\
&= \frac{\hbar^2}{2m} (2M\mathbf{n} + 2\mathbf{r}^\mu \partial_\mu) \\
&= \frac{i\hbar}{m} \mathbf{p}.
\end{aligned} \tag{25}$$

GEOMETRIC MOMENTUM DISTRIBUTION OF SPHERICAL HARMONICS The third aim of the present study is to give the probability distribution of geometric momentum of the spherical harmonics $Y_{lm}(\theta, \varphi)$. For our propose, we firstly give GM for particle on the surface of unit sphere.^{9,16,17}

$$p_x = -i\hbar(\cos \theta \cos \varphi \frac{\partial}{\partial \theta} - \frac{\sin \varphi}{\sin \theta} \frac{\partial}{\partial \varphi} - \sin \theta \cos \varphi), \tag{26}$$

$$p_y = -i\hbar(\cos \theta \sin \varphi \frac{\partial}{\partial \theta} + \frac{\cos \varphi}{\sin \theta} \frac{\partial}{\partial \varphi} - \sin \theta \sin \varphi), \tag{27}$$

$$p_z = i\hbar(\sin \theta \frac{\partial}{\partial \theta} + \cos \theta). \tag{28}$$

These operators satisfy the definition of the vector operator¹⁸ as $[L_i, p_j] = i\hbar \varepsilon_{ijk} p_k$, we can therefore have the operators p_x and p_y from p_z by means of rotation of the axis' rotation. Explicitly, rotation $\pi/2$ around y -axis renders p_z to be p_x , and $-\pi/2$ around x -axis renders p_z to be p_y ,

$$p_x = \exp(-i\pi L_y/2) p_z \exp(i\pi L_y/2), \quad p_y = \exp(i\pi L_x/2) p_z \exp(-i\pi L_x/2). \tag{29}$$

Here we follow the convention that a rotation operation affect a physical system itself.¹⁸ Hence the eigenvalue problem for operators p_x or p_y is simultaneously determined once the complete solution to $\hat{p}_z \psi_{p_z}(\theta) = p_z \psi_{p_z}(\theta)$ is known, where on operator p_z on the left hand side of this equation the carat symbol " ^ " is used to distinguish the eigenvalue p_z on the right hand side. The eigenfunctions $\psi_{p_z}(\theta)$ form a complete set once the eigenvalues p_z are real and continuous,

$$\psi_{p_z}(\theta) = \frac{1}{2\pi} \frac{1}{\sin \theta} \tan^{-ip_z} \left(\frac{\theta}{2} \right). \tag{30}$$

They are δ -function normalized,

$$\begin{aligned}
& \oint \psi_{p'_z}^* (\theta, \varphi) \psi_{p_z} (\theta, \varphi) \sin \theta d\theta d\varphi \\
&= \frac{1}{2\pi} \int_0^\pi \exp \left(i (p'_z - p_z) \left(\ln \tan \frac{\theta}{2} \right) \right) \frac{1}{\sin \theta} d\theta \\
&= \frac{1}{2\pi} \int_0^\pi \exp \left(i (p'_z - p_z) \ln \tan \frac{\theta}{2} \right) d \ln \tan \frac{\theta}{2} \\
&= \frac{1}{2\pi} \int_{-\infty}^\infty \exp (i (p'_z - p_z) z) dz \\
&= \delta (p'_z - p_z),
\end{aligned} \tag{31}$$

where the variable transformation $\ln \tan \theta/2 \rightarrow z$ is used. So, we see explicitly that the eigenfunctions $\psi_{p_z}(\theta)$ form a complete set. Next we use it to expand the spherical harmonics $Y_{lm}(\theta, \varphi)$. Because of the symmetry, the momentum distribution along z -axis depends on the angular quantum number l only. The result turns out to be,

$$\begin{aligned}
\varphi_l(p_z) &= \oint Y_{lm}(\theta, \varphi) \psi_{p_z}^* (\theta, \varphi) \sin \theta d\theta d\varphi \\
&= \sqrt{\frac{2l+1}{2}} F(p_z) \left[\frac{P_l(\tanh q)}{\cosh q} \right],
\end{aligned} \tag{32}$$

where P_l is the Legendre function of order l and the Fourier transform $F(p) [f(q)]$ of a function $f(q)$ is defined by,

$$F(p) [f(q)] \equiv \int f(q) \frac{e^{-ipq}}{\sqrt{2\pi}} dq. \tag{33}$$

The first three momentum distribution $\varphi_l(p_z)$ are respectively,

$$\varphi_0(p_z) = \frac{\sqrt{\pi}}{2} \sec h \left(\frac{\pi p_z}{2} \right), \tag{34}$$

$$\varphi_1(p_z) = \frac{i\sqrt{3\pi}}{2} p_z \sec h \left(\frac{\pi p_z}{2} \right), \tag{35}$$

$$\varphi_2(p_z) = \frac{\sqrt{5\pi}}{8} (3p_z^2 - 1) \sec h \left(\frac{\pi p_z}{2} \right). \tag{36}$$

The ground state $Y_{00}(\theta, \varphi)$ is the minimum uncertainty state for three pairs of (x_i, p_i) and $\Delta x_i \Delta p_i = \hbar/3$. In zero angular momentum state $Y_{00}(\theta, \varphi)$ that bears no energy either, the presence of zero-point the momentum fluctuation $\overline{(\Delta p_i)^2} = \hbar^2/3$ contradicts what classical mechanics would indicate. In overall respects, these states bears striking resemblance to the probability amplitude of the momentum for one-dimensional simple harmonic oscillator.

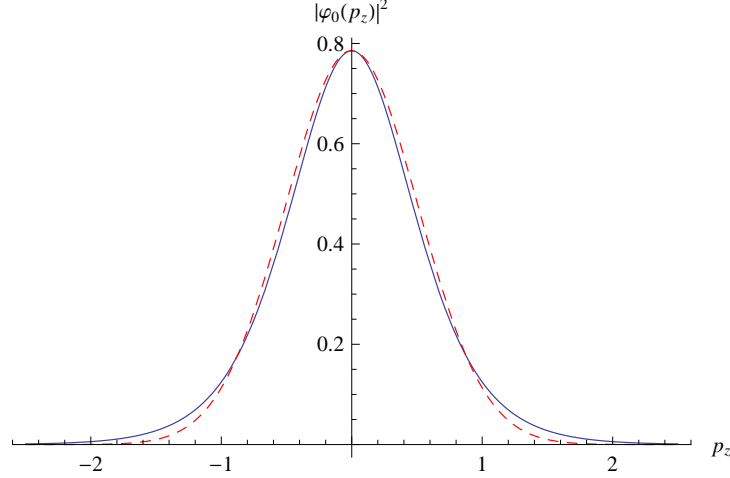


FIG. 1. Momentum distribution density for $Y_{00}(\theta, \varphi)$ (solid line) and for the ground state of 1D simple harmonic oscillator (dashed line) are plotted. They are almost identical.

The momentum distributions in the spherical harmonics offers an experimentally testable result for rotational state of spherical molecule such as C_{60} . With preparing these molecules into ground state of rotation, the probability of the momentum distributions is depicted in Fig. 1.

CONCLUSIONS AND DISCUSSIONS By use of the same confining procedure pioneered by Jensen, Koppe² and da Costa³ to give the geometric potential, we find that the momentum $\mathbf{p} = -i\hbar\nabla$ originally defined in bulk becomes a momentum $\mathbf{p} = -i\hbar(\mathbf{r}^\mu\partial_\mu + M\mathbf{n})$ (5) defined on the surface, which was previously proposed on completely different ground. Remarkably, this momentum is compatible with the Dirac's canonical quantization theory on system with second-class constraints. Because $\mathbf{r}(q^1, q^2)$ (6) in mathematics offers the so-called standard parametrization of the 2D surface, the corresponding momentum \mathbf{p} (5) should be also preferable over other forms of momentum such as the generalized momenta (p_{q^1}, p_{q^2}) canonically conjugated to parameters (q^1, q^2) . This is another reason it deserves a terminology, *geometric momentum* as we called. The distribution amplitudes of the geometric momentum of the spherical harmonics are analytically determinable, and experimentally testable for rotational state of spherical molecule such as C_{60} .

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